Simulating granular materials in LS-DYNA using Discrete Element Spheres (DES)

Outline

- Introduction
  - Motivation of DES
  - Principle of DES simulations

- Creating a keyword deck
  - Nodes and elements
  - Generating and de-activating particles
  - Particle to particle contact
  - Particle to structure contact

- Post-processing
  - Spherical representation of DES
  - Wear
  - DES as points

- Summary of relevant keywords

Why simulations with DES?

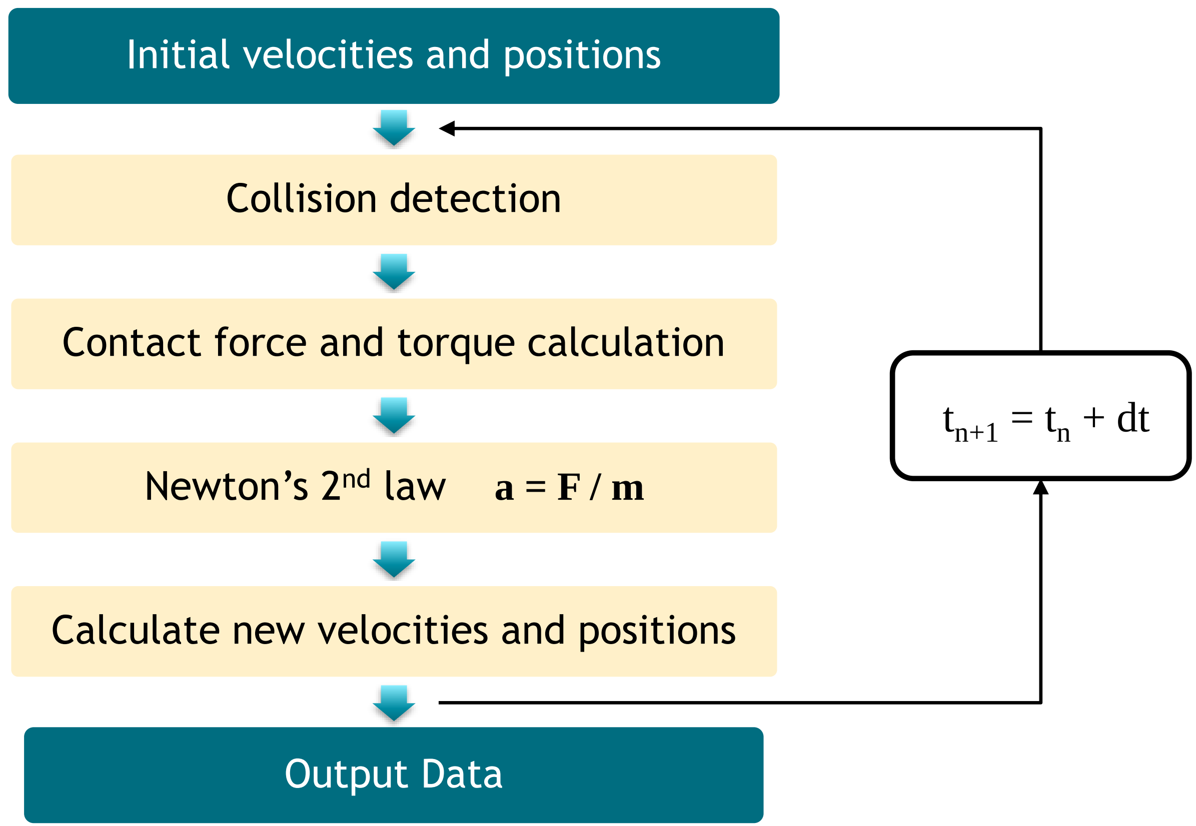
- Granular materials are not easily described as fluids, nor are they easily described as solids.
- Jelly beans, sesamy seeds, coffee beans, sand, coarse gravel, medical pills, fertilizers, coal …
- Numerical simulations could help in the design of:
  - Storage
    - Silos, Piles
  - Transportation
    - Conveyor belts, screws, pumps, trucks
  - Processing
    - Sorting, mixing, segregation
  - Filling
    - Hopper/funnel flow, packaging
  - …

Why simulations with DES?

- By using simulations with DES, it is possible to assess e.g.
  - bulk flow capacities
  - loads from the granular media on structures
  - wear induced by the material handling
  - load on granular media
  - …

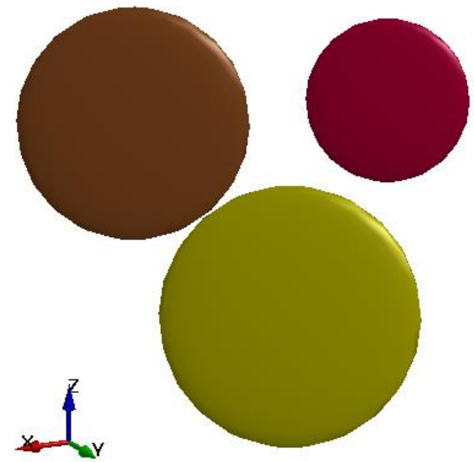
Principle of DES simulations

- The rigid spherical particles with mass, radius and six degrees of freedom, follow Newton's laws of motion and interact through contact.



DES – The elements

- Input the size and position of each particle.



$$M = V\rho = \frac{4}{3}\pi r^3 \rho \qquad I = \frac{2}{5} M r^2 = \frac{8}{15}\pi r^5 \rho$$

```
*ELEMENT_DISCRETE_SPHERE_{OPTION}
$---+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
$#     NID       PID      MASS   INERTIA    RADIUS
     30001         4  570.2710  6036.748      5.14
     30002         5  399.0092  3328.938      4.57
     30003         6  139.1240   575.004      3.21
*NODE
$--+---1-------+-------2-------+-------3-------+-------4---+---5---+---6
$#   NID               X               Y               Z      TC      RC
   30001          -29.00           -26.8             8.7       0       0
   30002          -21.00           -24.8            18.2       0       0
   30003          -27.00           -14.7            21.2       0       0
```

DES – The elements

- Density can be set to unity in generation of particles, and the properties can be scaled later using e.g. *MAT_ELASTIC.

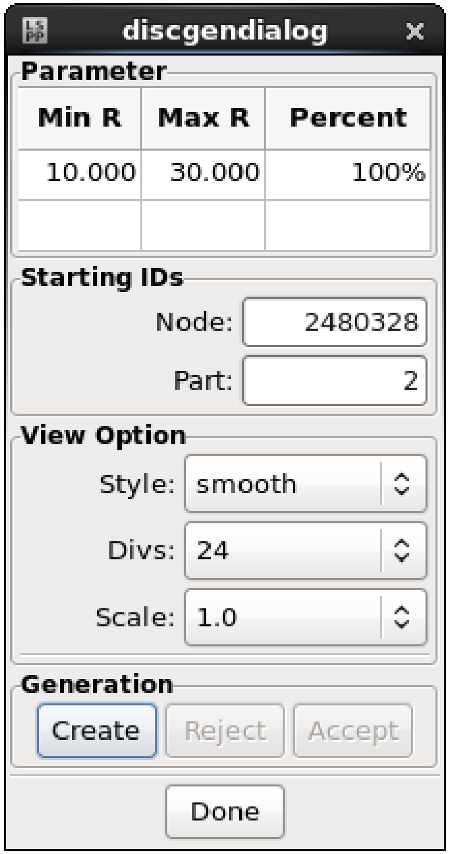
(i.e., by using the _VOLUME option, it is not the actual mass and inertia that is presented in the *ELEMENT_DISCRETE_SPHERE_VOLUME keyword.)

$$M = V\rho = \frac{4}{3}\pi r^3 \rho \qquad I = \frac{2}{5} M r^2 = \frac{8}{15}\pi r^5 \rho$$

```
*ELEMENT_DISCRETE_SPHERE_VOLUME
$---+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
$#      NID         PID        MASS   INERTIA     RADIUS
      30001           4   570.2710  6036.748       5.14
      30002           5   399.0092  3328.938       4.57
      30003           6   139.1240   575.004       3.21
*NODE
$--+---1-------+-------2-------+-------3-------+-------4---+---5---+---6
$#    NID                X               Y               Z      TC      RC
    30001           -29.00           -26.8             8.7       0       0
    30002           -21.00           -24.8            18.2       0       0
    30003           -27.00           -14.7            21.2       0       0
```

Generating packed particles in LS-PrePost

- Automatic packing algorithm for meshed objects.
  - Bounded volume is required with 3- or 4-noded elements.
  - Support for double-connected volumes, mesh for inner and outer surface needed.
  - Surface normals need to be consistent.
  - Supports distribution of radii.
  - Single-thread implementation.
  - Available from LS-PrePost v4.2.

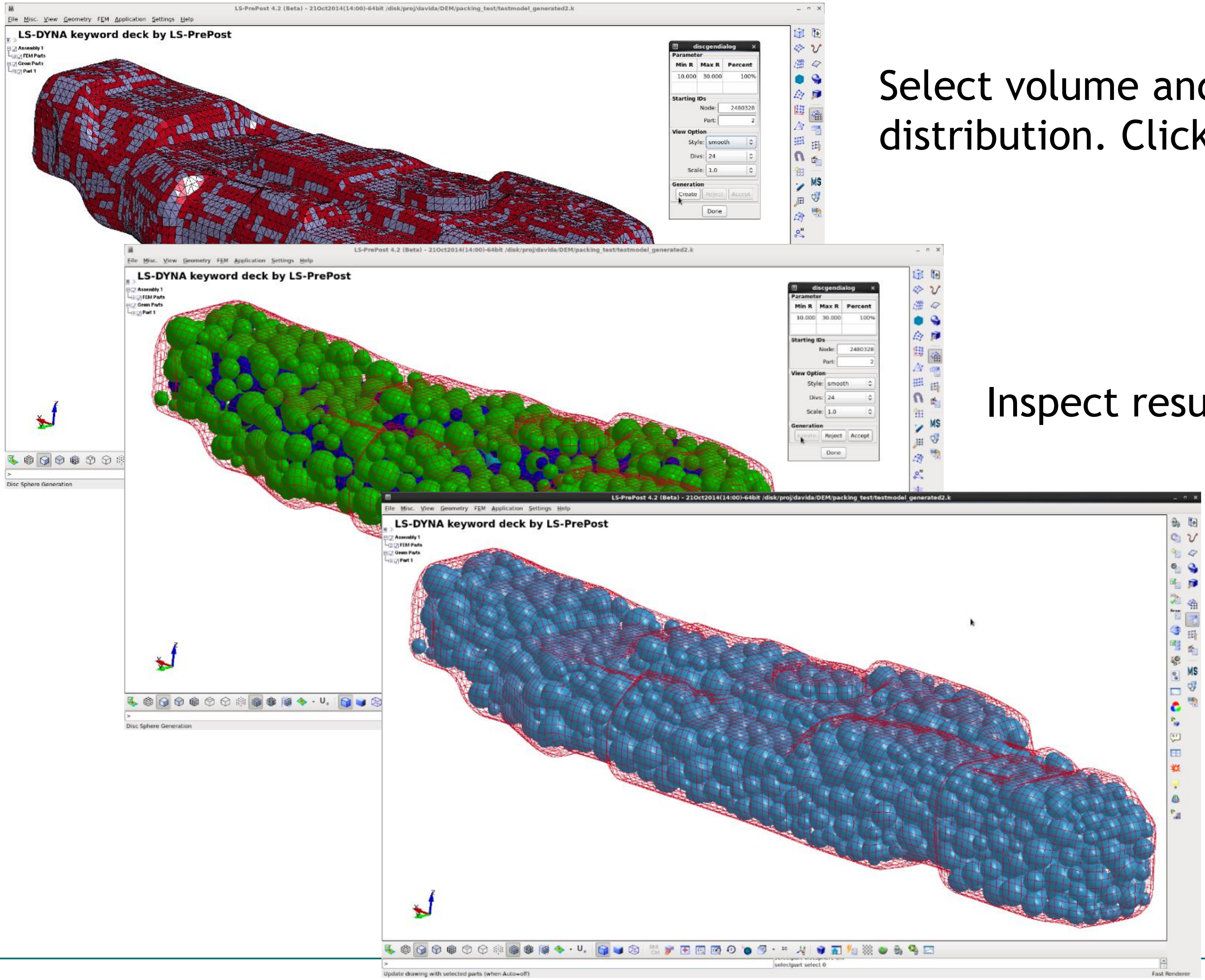


Particles are not completely packed afterwards. Optionally, perform a simulation with gravity and possibly vibrational loading to allow particles to settle.

After generation, use the _VOLUME option, since the generated particles have a density equal to unity.

Shell thickness is not accounted for in packing algorithm!

Generating packed particles in LS-PrePost – procedure



Select volume and set radius distribution. Click create.

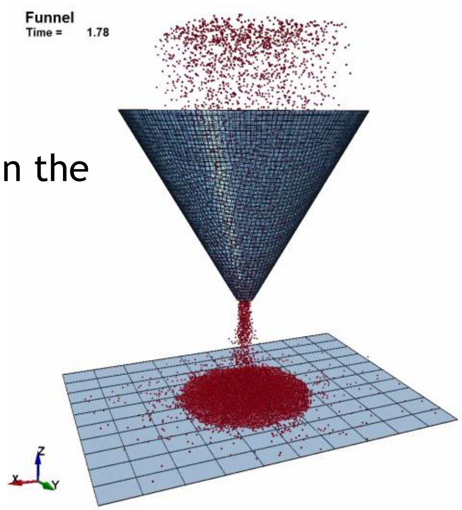
Inspect results and accept.

View final result.

Automatic particle generation in LS-DYNA

```
*DEFINE_DE_INJECTION_OPTION
$---+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
$#     pid       sid        xc        yc        zc        xl        yl       cid
         2         1       0.0       0.0     600.0     300.0     400.0
$#   rmass      rmin      rmax        vx        vy        vz      tbeg      tend
    0.0005       1.0       3.0                                               2.0
$#   ifunc       nid    imulti      lcvx      lcvy      lcvz
         0         0         1         0         0         0
$# Included when imulti > 1
$#      r1        p1        r2        p2        r3        p3        r4        p4
         0         0         0         0         0         0         0         0
```

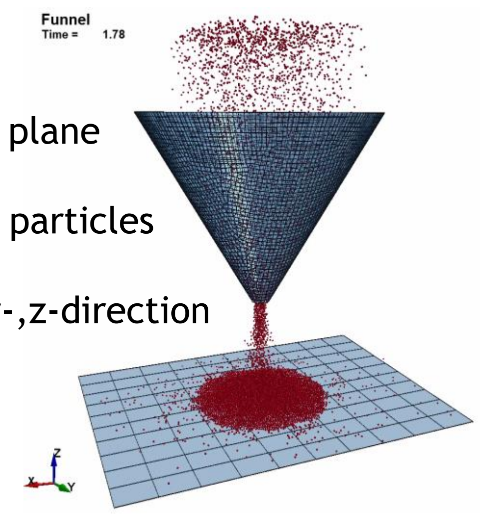
PID	Part ID of new generated DES nodes
SID	Node set ID of new generated DES nodes
XC, YC, ZC	X,Y,Z coordinate of the center of the injection plane
XL, YL	Length of rectangular injection plane along X- & Y-axis in the global or local coordinate system (if CID is defined)
CID	Optional local coordinate system ID
RMASS	Mass flow rate
RMIN	Minimum DES radius
RMAX	Maximum DES radius
VX, VY, VZ	Vector components defining the initial velocity of injected DES in the defined coordinate system (CID)



Automatic particle generation in LS-DYNA

```
*DEFINE_DE_INJECTION_OPTION
$---+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
$#      pid       sid        xc        yc        zc        xl        yl       cid
          2         1       0.0       0.0     600.0     300.0     400.0
$#    rmass      rmin      rmax        vx        vy        vz      tbeg      tend
     0.0005       1.0       3.0                                                2.0
$#    ifunc       nid    imulti      lcvx      lcvy      lcvz
          0         0         1         0         0         0
$# Included when imulti > 1
$#       r1        p1        r2        p2        r3        p3        r4        p4
          0         0         0         0         0         0         0         0
```

TBEG	Birth time
TEND	Death time
IFUNC	Distribution for particle sizes, uniform or gaussian
NID	An optional node ID. If defined, the center of injection plane follows the motion of this node.
IMULTI	Flag for giving a specified mass distribution of injected particles with given radii.
LCVX,LCVY,LCVZ	Load curve defining initial injection velocity in the x-,y-,z-direction
Ri	Injected particle radius
Pi	Mass percentage of injected particle with radius Ri



Automatic particle generation in LS-DYNA

```
*DEFINE_DE_INJECT_BONDED
$---+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
$#      pid       sid        xc        yc        zc        xl        yl       cid
                            0.0       0.0       0.0       0.0       0.0         0
$#    rmass        vx        vy        vz      tbeg      tend
                  0.0       0.0       0.0       0.0    1.0e20
$#      pbn       pbs     pbn_s     pbs_s       sfa     alpha    maxgap
                            0.0       0.0       1.0       0.0    1.0e-4
$#   nshape
          0
$#   Additional cards for NSHAPE!=0
$#   ishape    ishape    ishape    ishape    ishape    ishape    ishape    ishape
```

New from R11

This keyword injects bonded discrete element spheres (DES) from a specified region at a flow rate given by a user defined curve.

Like *DEFINE_DE_INJECTION, when the option is blank, the region from which the DES emanate is assumed rectangular; the ELLIPSE option indicates that the region is elliptical.

The first two cards are very similar to *DEFINE_DE_INJECTION.

Automatic particle generation in LS-DYNA

```
*DEFINE_DE_INJECT_SHAPE
$---+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
$#      id       nde

$#       x         y         z         r
```

New from R11

Purpose: Define the bonded shape patterns.

When used with *DEFINE_DE_INJECT_BONDED, these shape patterns will be injected with equal probability. Each pattern contains several DEs, and the pattern can be in any direction. The relative positions and radii of DEs should be calculated correctly in order to generate bonds between the neighboring DEs; see the field MAXGAP in *DEFINE_DE_INJECT_BONDED.

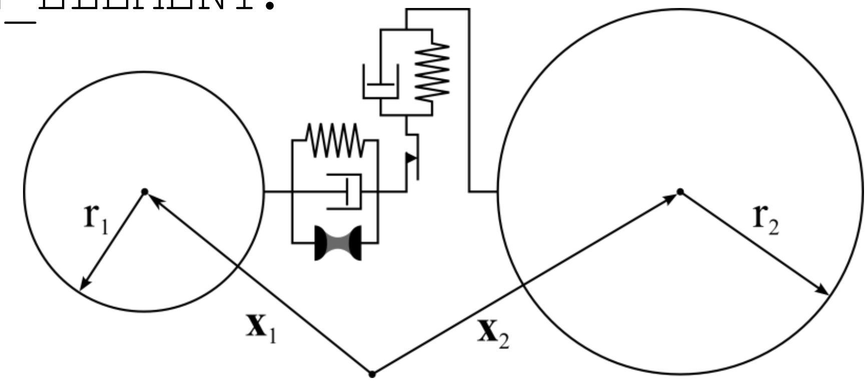
DES – material and section

- The element type and formulation values in *SECTION are ignored.
- LS-DYNA retrieves the bulk modulus from the *MAT input for coupling stiffness and time step size evaluation in a DES simulation, and density from the *MAT input if VOLUME is used to calculate the proper mass. *MAT_ELASTIC and *MAT_RIGID are most commonly used, but other material models are also permissible.

```
*SECTION_SOLID
$---+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
$#   SECID    ELFORM       AET
         4         0         0
*MAT_RIGID
$---+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
$#     MID        RO         E        PR         N    COUPLE         M     ALIAS
         4   2.65E-9     50000      0.24       0.0       0.0       0.0
$#     CMO      CON1      CON2
       0.0         0         0
$#LCO OR A1       A2        A3        V1        V2        V3
       0.0       0.0       0.0       0.0       0.0       0.0
```

DES to DES interactions

- Interactions between discrete elements are controlled by the global keyword `*CONTROL_DISCRETE_ELEMENT`.

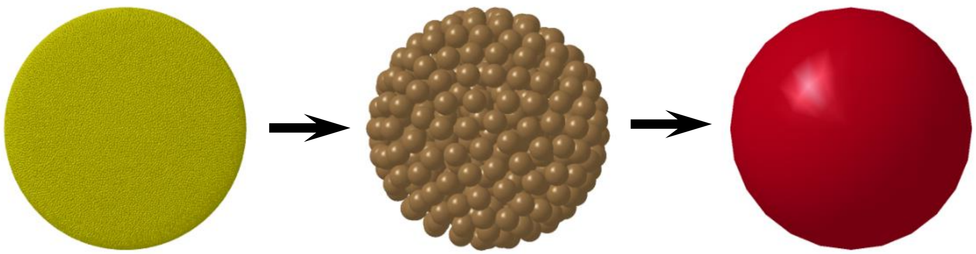



```
*CONTROL_DISCRETE_ELEMENT
$---+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
$#    NDAMP     TDAMP     FRICS     FRICR     NORMK    SHEARK       CAP       VTK
      0.700     0.400      0.41     0.001      0.01    0.0029         0         0
$#    GAMMA       VOL       ANG       GAP              IGNORE      NBUF  PARALLEL
       26.4      0.66      10.0         0                   0         6         0
$#    LNORM    LSHEAR               FRICD        DC                  BT        DT
          0         0                0.41         0                  0.     10e20
```

- DES properties can also be set on part level by using `*DEFINE_DE_BY_PART`. Those settings override `*CONTROL_DISCRETE_ELEMENT`.

Modelling – Coarse graining

- Scenario – real particles small
  - Coarse-graining needs to be applied depending on the available computer power (also known as “upscaling”, e.g. *Feng* et al. 2009)



546 820 spheres with $r_{\text{real}} = 0.01$ | 491 spheres with $r_{\text{real}} = 0.1$ | 1 sphere with $r_{\text{bulk}} = 1.0$

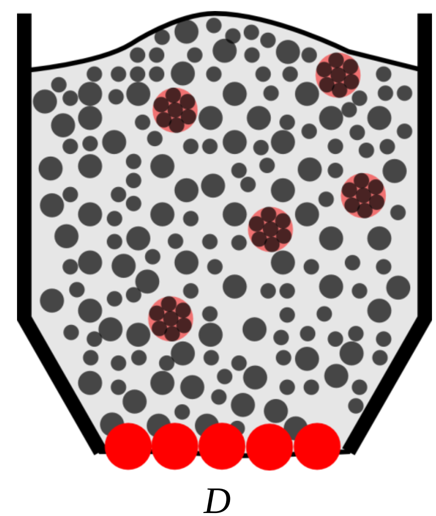
  - Scale number S_{n} to characterize coarse-graining

$$S_{\text{n}} = \frac{D}{r_{\text{bulk}}} \geq 10 \qquad \begin{cases} D & \text{: characteristic length (e.g. outlet)} \\ r_{\text{bulk}} & \text{: coarse-grained bulk radius} \end{cases}$$

  - Bulk vs. real particle density

$$\rho^{\text{bulk}} = n\,\rho^{\text{particle}} \quad \text{with } n \text{ : porosity}$$

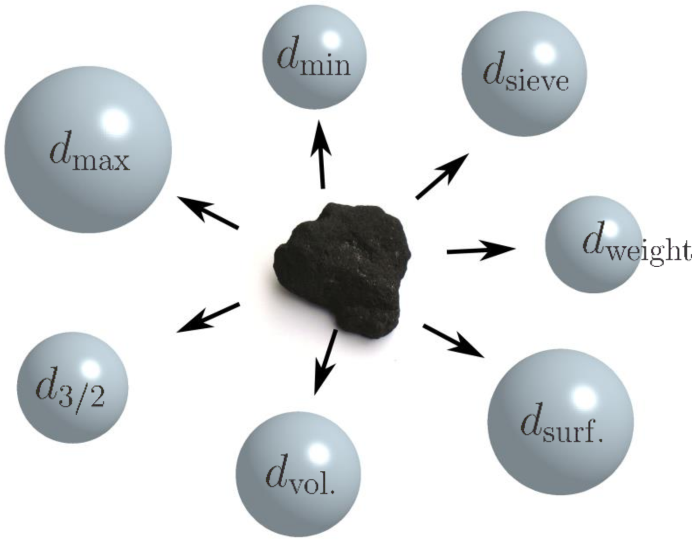
- Things to keep in mind
  - Several particles are represented by a single (rigid) particle
  - Interaction behavior needs to be derived from bulk experiments



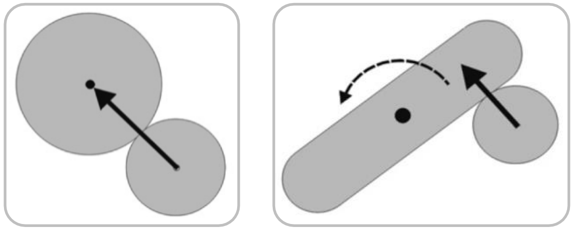
Modelling – Non-spherical particles

- Scenario – real particles large
  - Spherical particles: Measure radius
  - Non-spherical particles: Equivalent sphere approximation
    - Define average radius based on same
      - minimal/maximal diameter
      - sieve size diameter
      - surface, volume, weight
    - Sauter mean diameter [*Sauter* 1926]

$$d_{3/2} = \frac{d^3_{\text{vol.}}}{d^2_{\text{surf.}}} = \frac{6\,V_{\text{part.}}}{A_{\text{part.}}} \qquad \begin{cases} d_{\text{vol.}} & = \left(\dfrac{6\,V_{\text{part.}}}{\pi}\right)^{1/3} \\ d_{\text{surf.}} & = \sqrt{\dfrac{A_{\text{part.}}}{\pi}} \end{cases}$$

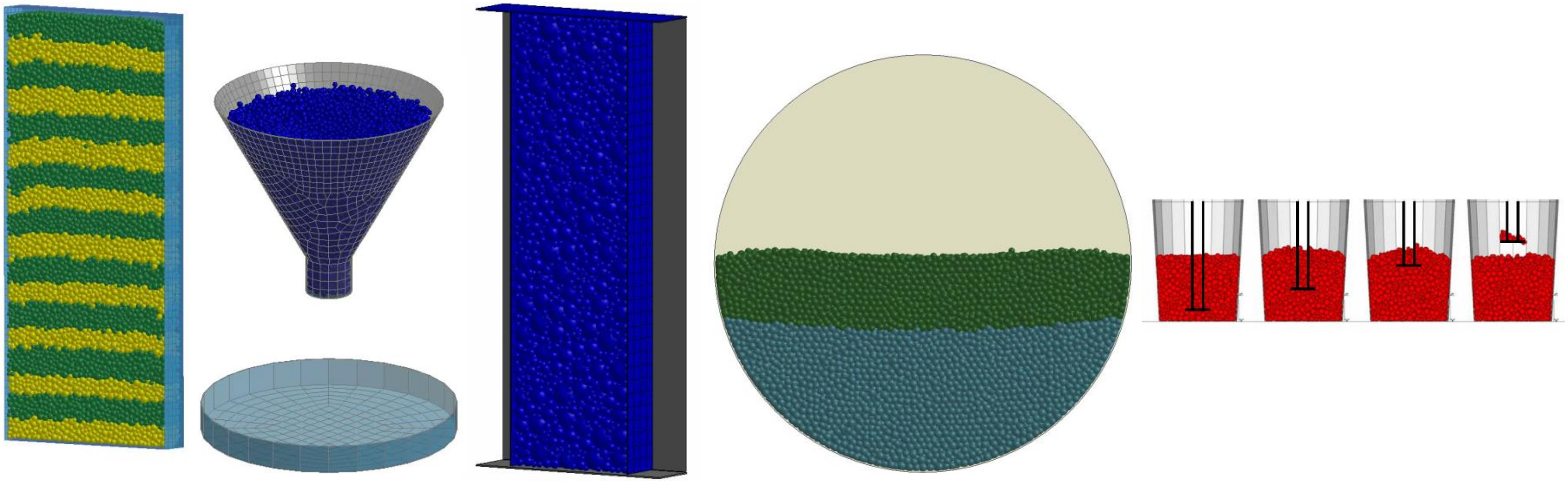


- Things to keep in mind
  - Non-spherical particles introduce moments due to an offset of contact forces!



Calibration of DES parameters

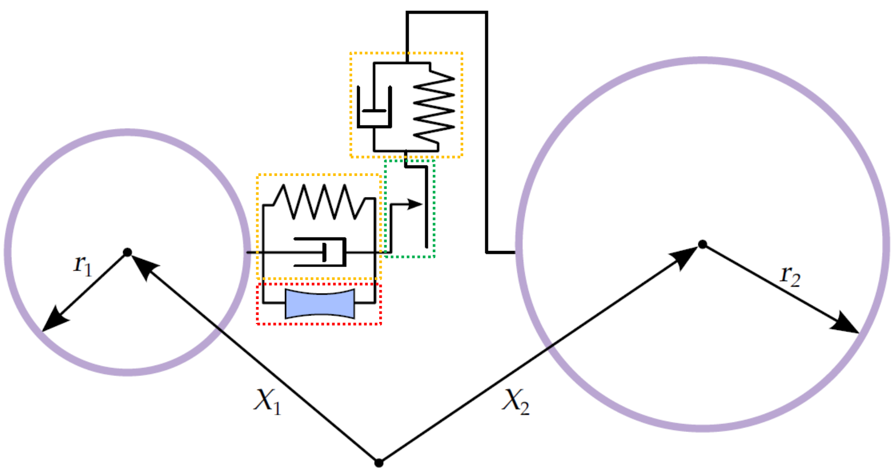
- Calibration of the DES to DES interaction parameters can e.g. be made through inverse modelling of bulk experiments.

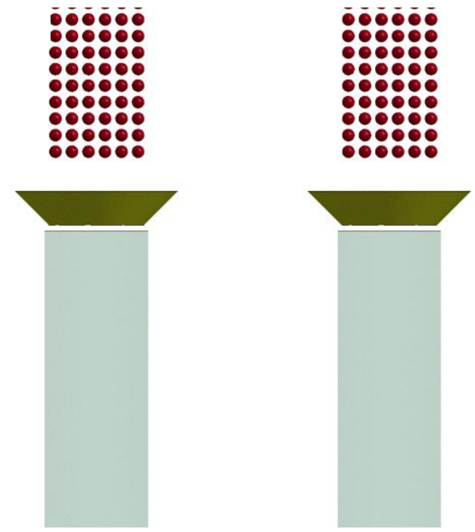


Parameters to calibrate

```
*CONTROL_DISCRETE_ELEMENT
$---+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8
$#   NDAMP     TDAMP     FRICS     FRICR     NORMK    SHEARK       CAP       VTK
     0.700     0.400      0.41     0.001      0.01    0.0029         0         0
$#   GAMMA       VOL       ANG       GAP              IGNORE      NBUF  PARALLEL
      26.4      0.66      10.0         0                   0         6         0
$#   LNORM    LSHEAR               FRICD        DC      NCRB        BT        DT
         0         0                0.41         0         0        0.    10e20
```

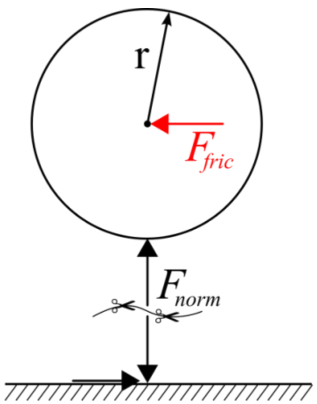
- Friction parameters.
- Contact damping and stiffness.
- Capillary forces parameters.



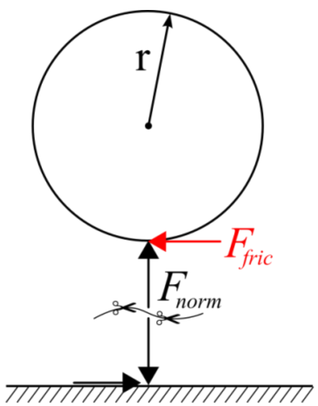


wet dry

Contact DES to surface



Classic contact



New DE contact

FricS = friction coefficient
FricD = rolling friction coefficient

***DEFINE_DE_TO_SURFACE_COUPLING**

Purpose: To define a non-tied coupling interface between discrete element spheres (DES) and a surface defined by shell part(s) or solid part(s). This coupling is currently not implemented for tshell part(s).

Card 1	1	2	3	4	5	6	7	8
Variable	SLAVE	MASTER	STYPE	MTYPE				
Type	I	I	I	I				
Default	0	0	0	0				

Card 2	1	2	3	4	5	6	7	8
Variable	FricS	FricD	DAMP	BSORT	LCVx	LCVy	LCVz	WEARC
Type	F	F	F	I	I	I	I	F
Default	0	0	0	100	0	0	0	0.

User Defined Wear Parameter Cards. Additional Card for WEARC.LT.0.

Card 3	1	2	3	4	5	6	7	8
Variable	W1	W2	W3	W4	W5	W6	W7	W8
Type	F	F	F	F	F	F	F	F
Default	none	none	none	none	none	none	none	none

Card 4 is optional.

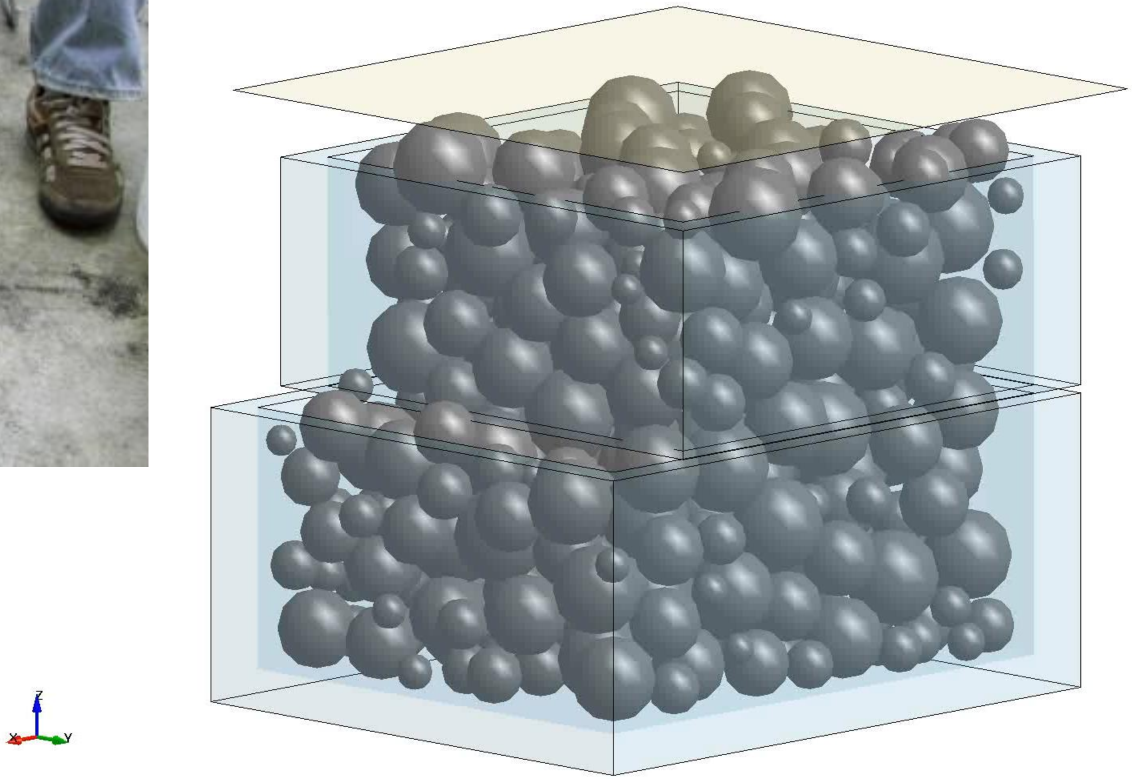
Card 4	1	2	3	4	5	6	7	8
Variable	SFP	SFT				CID_RCF	BT	DT
Type	F	F				I	F	F
Default	1.0	1.0				0	0	1.E20

- Friction force is applied at the perimeter.
- Possibility to define transportation belt velocity via `LCV`.
- Optional calculation of wear using Archard's wear law, Finnie's wear law or user defined wear law.

Example – Calibration of frictional parameters for coarse gravel

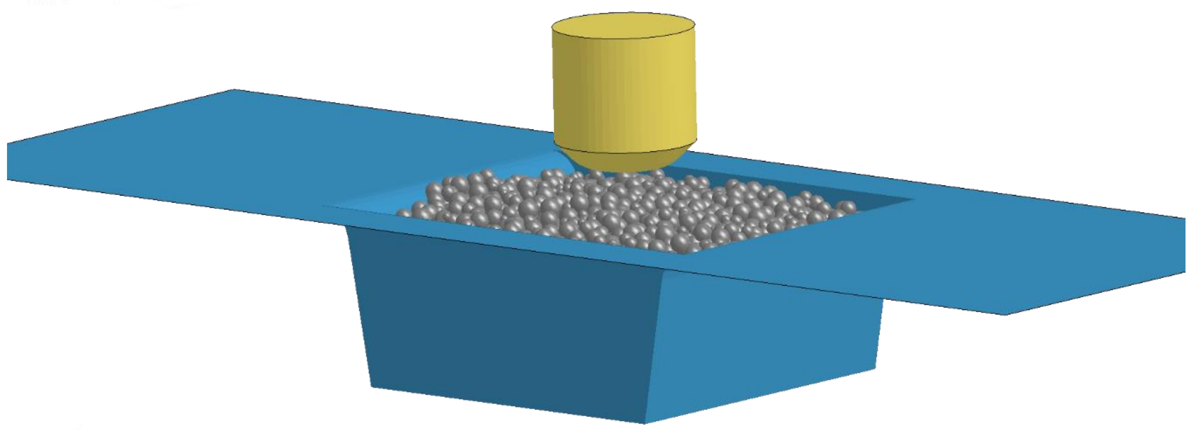
- The shear box test

Huang G., *Discrete element modeling of railroad ballast using imaging based aggregate morphology characterization*, Disseratation, University of Illinois at Urbana-Champaign, 2010.



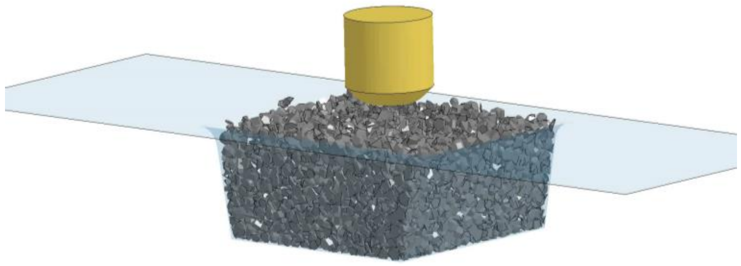
Dynamic load case 1: Drop test

- Box dimensions: Length 1200 mm, width 1000 mm, depth 500 mm
- Cylinder: Mass 780 kg, initial velocity 4 m/s
- SDEM: Particle size 20 – 60 mm, static friction 0.8
- Friction coefficient of box and cylinder: 0.16

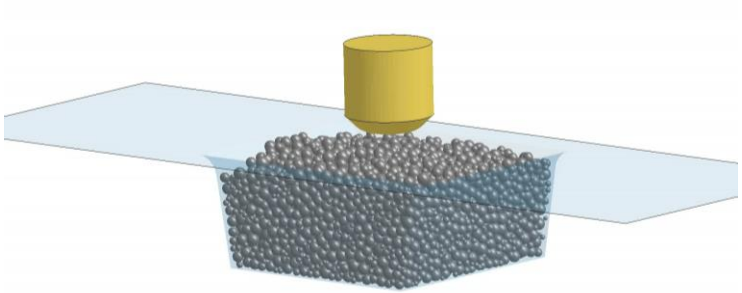


Dynamic load case 1: Drop test

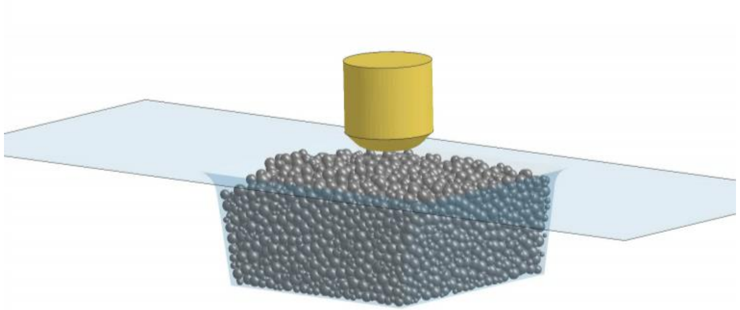
Frics: 0.6



Frics: 0.8
Fricr: 0.0

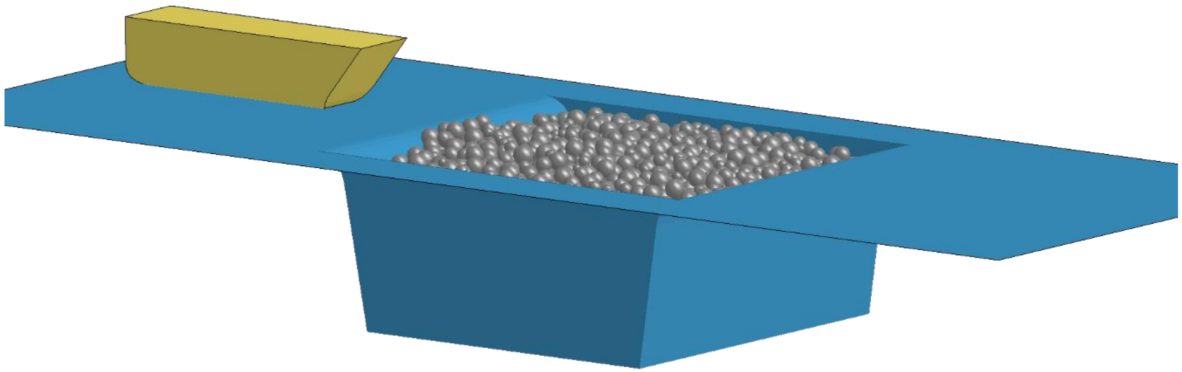


Frics: 0.8
Fricr: 0.6



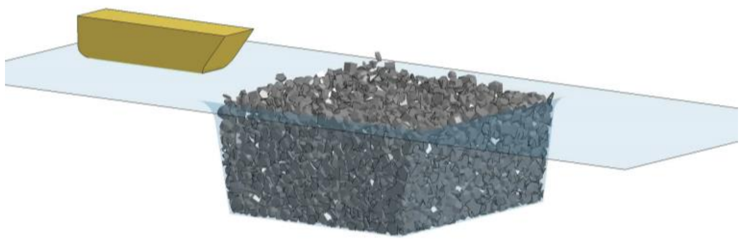
Dynamic load case 2: Slide test

- Box dimensions: Length 1200 mm, width 1000 mm, depth 500 mm
- Rigid body: Mass 2500 kg, prescribed velocity 1 m/s
- SDEM: Particle size 20 – 60 mm, static friction 0.8
- Friction coefficient of box and rigid body: 0.16

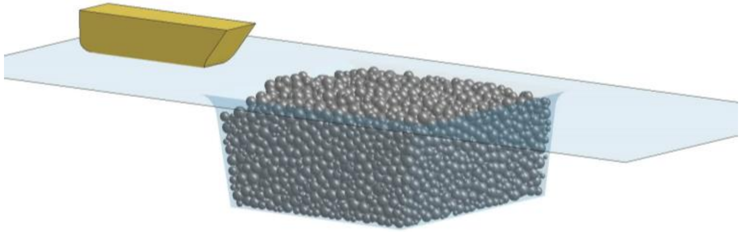


Dynamic load case 2: Slide test

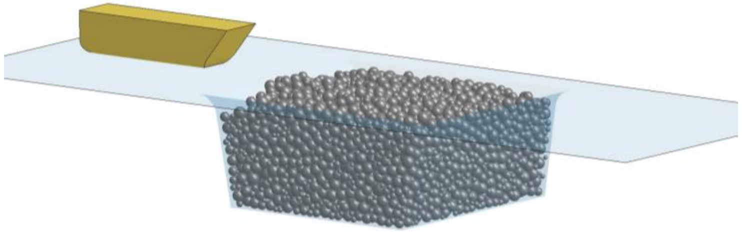
Frics: 0.6



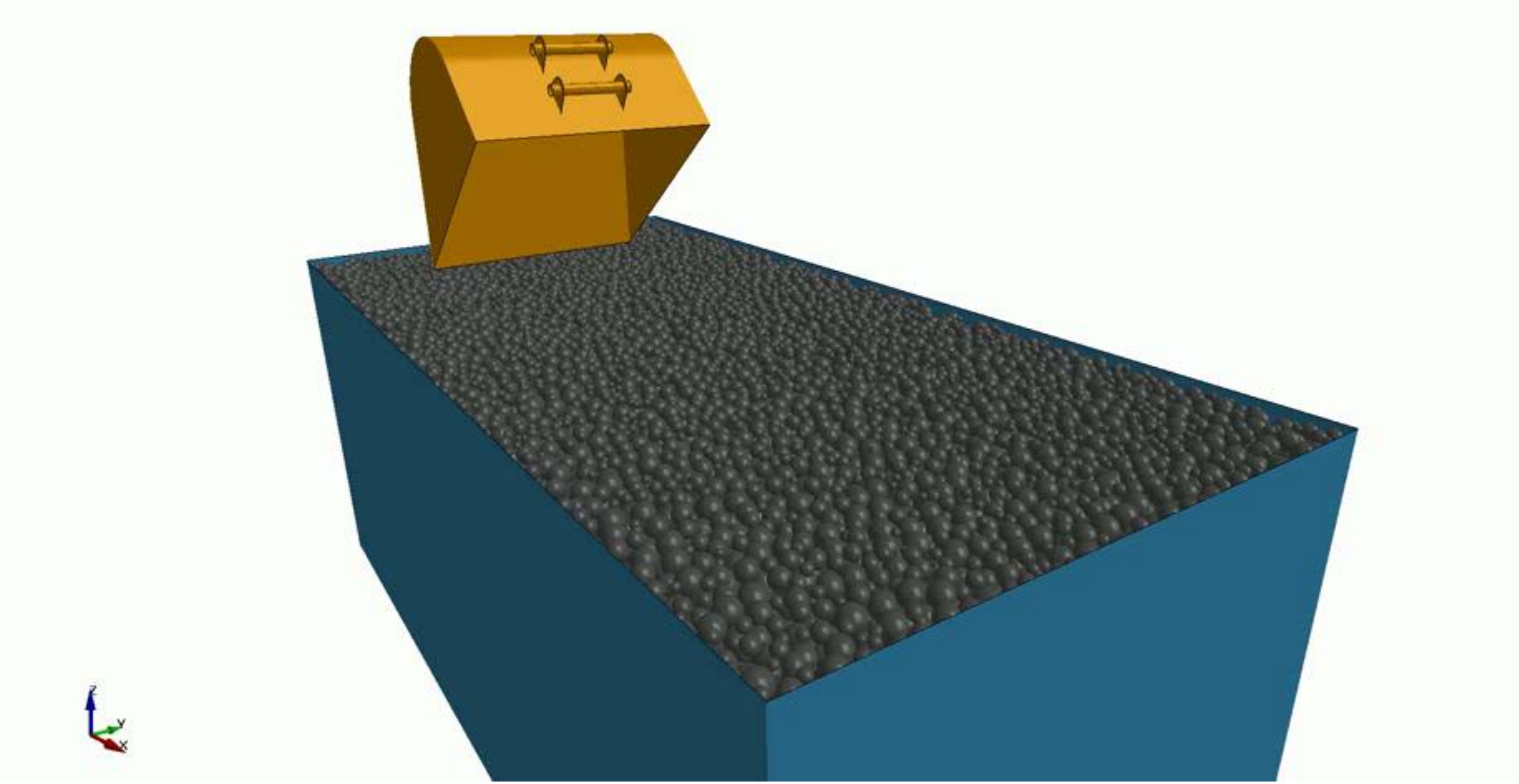
Frics: 0.8
Fricr: 0.0



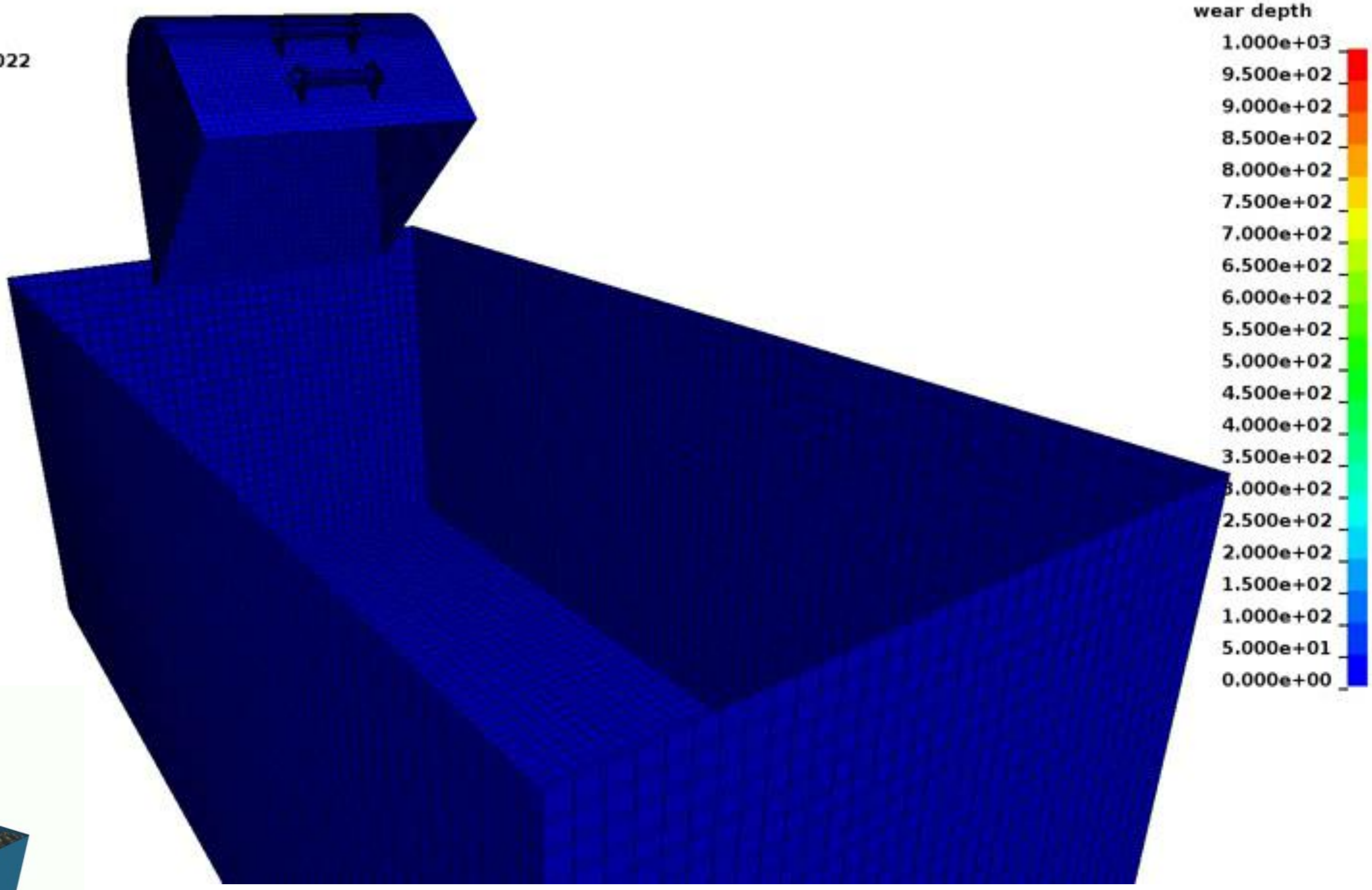
Frics: 0.8
Fricr: 0.6

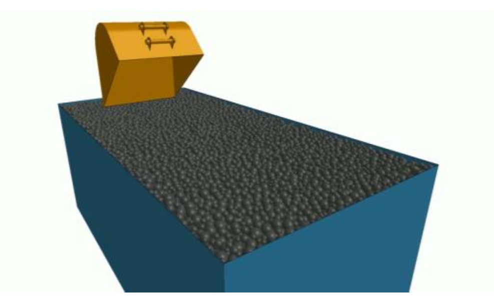


Example: Excavation bucket

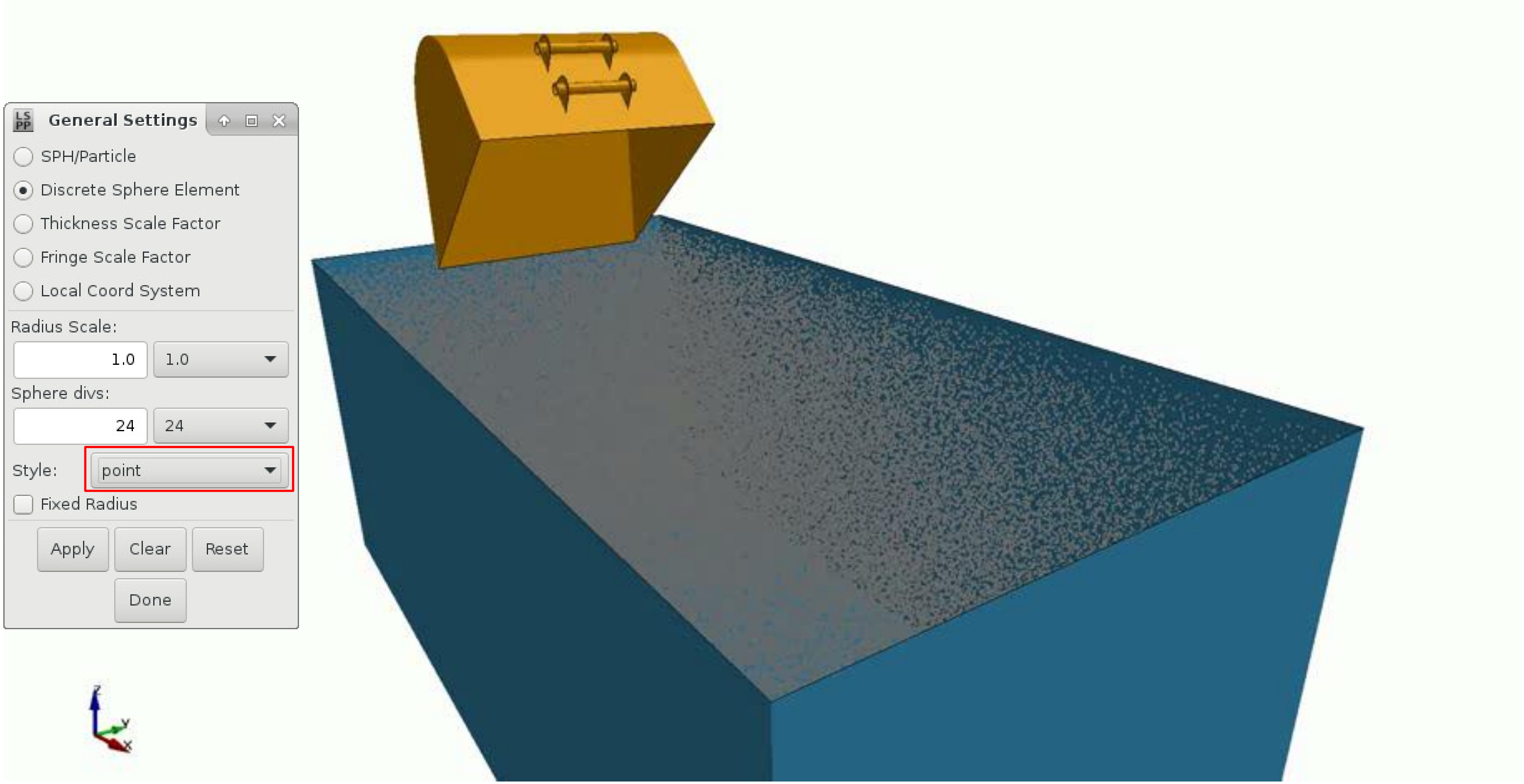


Post-processing – Wear (*DATABASE_BINARY_DEMFOR)





Post-processing – DES as points



Summary of involved keywords

- Manual definition of DES with pre-processor
  - ***NODE**
    - Gives the location of the particle
  - ***ELEMENT_DISCRETE_SPHERE_OPTION**
    - Element ID, mass, inertia and radius of the particle
- Automatic generation of DES
  - ***DEFINE_DE_INJECTION_OPTION**
    - Generate a flow of DES without prior definition with ***ELEMENT_DISCRETE_SPHERE**
    - This saves CPU time as well as memory
    - The injection geometry is a rectangular plane
- Boundary conditions for DES
  - ***BOUNDARY_DE_NON_REFLECTING**
    - Non reflecting boundary conditions to prevent for instance stress wave reflections in half-space models

Summary of involved keywords

- Particle-particle interaction
  - ***CONTROL_DISCRETE_ELEMENT**
    - Global settings of coefficients for damping, friction, stiffness scaling & wet particles
  - ***DEFINE_DE_BY_PART**
    - Local settings of coefficients for damping, friction, stiffness scaling & wet particles
- Particle-structure interaction
  - ***DEFINE_DE_TO_BEAM_COUPLING**
    - Define contact between DEM spheres and Lagrangean beam parts
  - ***DEFINE_DE_TO_SURFACE_COUPLING**
    - Define contact between DEM spheres and Lagrangean structural parts
    - Setting coefficients for damping, friction, transportation and wear
  - ***DEFINE_DE_TO_SURFACE_TIED**
    - Tied contact between DEM spheres and Lagrangean structural parts
    - Setting tiebreak coefficients for failure

Summary of involved keywords

- ASCII Database for post-processing
  - ***DEFINE_DE_MASSFLOW_PLANE**
    - Define a plane across the mass flow rate of DES is measured
  - ***DATABASE_DEMASSFLOW**
    - Setting the output interval for the mass flow rate across the plane

- Binary Database for post-processing
  - ***DATABASE_BINARY_D3PLOT**
    - Setting the output interval for the binary d3plot file
    - Visualize contact force chains
    - Homogenized density
  - ***DATABASE_BINARY_DEMFOR**
    - Setting the output interval for the binary DEM coupling file
    - Visualize the particle-structure forces in the interface defined by ***DEFINE_DE_TO_SURFACE_COUPLING**
    - Visualize the wear depth on the Lagrangean surface
- Deactivate particles as they leave a defined volume
  - ***DEFINE_DE_ACTIVE_REGION**

Other keywords relevant for DES

*DEFINE_ADAPTIVE_SOLID_TO_DES

*DEFINE_DE_BOND

*DEFINE_DE_INJECT_BONDED

*DEFINE_DE_INJECT_SHAPE

*DEFINE_SPH_DE_COUPLING

*PARTICLE_BLAST

Thank you!

Your LS-DYNA distributor and more